Local quantum critical behavior in magnetic Kondo impurity models with partially screened moment

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In the strong coupling limit, an effective resonant level model is derived for the spin-1 underscreened Kondo impurity model. A local quantum critical behavior is induced by the formation of a bound state with partially screened magnetic moment, displaying a residual Z_2 symmetry, leading to a δ-resonance at the Fermi level in the impurity spectral function. As a consequence, a logarithmic singularity appears in the real part of the impurity dynamic spin susceptibility as a function of $\max(\omega, T)$, with ω as frequency, T temperature. A small magnetic field breaks this Z_2 symmetry and suppresses the singularity. We also discuss the possible manifestation of such a quantum critical behavior in the spin-1/2 two Kondo impurity model and the single quantum dot system with even electron occupation.

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I. INTRODUCTION

The Kondo model was initially introduced to describe the behavior of diluted magnetic impurities in metals, and has been thoroughly studied in various aspects. Localized quantum impurities also serve as building blocks of the heavy fermion materials, and there is still a strong interest in studying Kondo model on the lattice, particularly in view of the breakdown of Fermi liquid behavior due to incomplete Kondo screening close to a quantum critical point [1], as discovered in a large class of f-electron metals such as $CeCu_{6-x}Au_x$[2] and $YbRh_2Si_2$[3].

Recently, special attention was paid to the study of the underscreened Kondo problem which showed some evidence of deviation from the standard Fermi liquid behavior [4]. This result was interpreted as due to anomalous scattering of conduction electrons on a bound state with remaining unscreened magnetic moment. Although the large-N approaches using both spin-boson and spin-fermion representations were developed [5, 6], there are still some discrepancies between the obtained results. The more rigorous treatments based on the Bethe ansatz and numerical renormalization group (NRG) calculations lead to a "singular" Fermi liquid behavior [7, 8], namely a Fermi liquid fixed point with singular irrelevant corrections. However, these insightful works [7] mainly focused on the spinon phase shift and density of states, yielding *limited* results. In order to investigate the local dynamic singularity of the partially screened moment, we would like to propose a simple approach to grasp the essential physics of the strong coupling fixed point, revealing the origin of the singularity, and to explore the possible manifestation of such a quantum critical behavior in the spin-1/2 two Kondo impurity model and quantum dots with even electron occupation.

The paper is organized as follows. In Sec. II, we present our theory for the spin-1 underscreened Kondo impurity model. With a pseudo-fermion representation for the spin-1 operator, an effective resonant level model is derived in the strong coupling mean field (MF) approximation, and the static and dynamical properties of the effective model are given in detail. In Sec. III, a similar approach is proposed to treat the spin-1/2 two Kondo impurity model. From the resulting effective resonant level model, we identify that the two Kondo impurity model shares the same singular behavior as the spin-1 underscreened Kondo impurity model for the low-energy excitations. In Sec. IV, we also explore the possible realization of the singular underscreened Kondo behavior in a single quantum dot system with even number of electrons. The conclusion of the paper is given in Sec.V.

II. EXPLORATION OF THE SPIN-1 KONDO IMPURITY MODEL

The isotropic single Kondo impurity model is usually defined as:

$$H = \sum_{\mathbf{k},\sigma} \epsilon_{\mathbf{k}} C^{\dagger}_{\mathbf{k},\sigma} C_{\mathbf{k},\sigma} + \frac{J}{2}\left(S^{+} C^{\dagger}_{\downarrow} C_{\uparrow} + S^{-} C^{\dagger}_{\uparrow} C_{\downarrow}\right) + \frac{J}{2} S^{z}\left(C^{\dagger}_{\uparrow} C_{\uparrow} - C^{\dagger}_{\downarrow} C_{\downarrow}\right), \tag{1}$$

where $J > 0$ corresponds to an antiferromagnetic coupling. When the impurity spin $S > 1/2$, the strong coupling limit corresponds to formation of a bound state composed of the conduction electron and the magnetic moment [9]. Such a bound state would have a residual degeneracy associated with the remanent magnetic moment. It is believed that such a partially screened *quantum* moment should induce a local quantum critical behavior close to zero temperature [4].

A. Pseudo-fermion representation for spin-1 operator

As the simplest case, we consider a spin-1 magnetic impurity. Introducing a pseudo-fermion representation:

$$\begin{aligned} S^{+} &= \sqrt{2}\left(d_0^{\dagger}d_{-1} + d_1^{\dagger}d_0\right), \\ S^{-} &= \sqrt{2}\left(d_{-1}^{\dagger}d_0 + d_0^{\dagger}d_1\right), \\ S^{z} &= \left(d_1^{\dagger}d_1 - d_{-1}^{\dagger}d_{-1}\right), \end{aligned} \tag{2}$$

where d_1, d_0, d_{-1} correspond to the three components of $S^z = 1, 0, -1$, respectively. To fix the quantum spin magnitude of $S^2 = 2$, we have to impose the constraint

$$d_1^{\dagger}d_1 + d_0^{\dagger}d_0 + d_{-1}^{\dagger}d_{-1} = 1. \tag{3}$$

Since the commutation relations are obeyed $[S^+, S^-] = 2S^z$ and $[S^z, S^{\pm}] = \pm S^{\pm}$ forming an SU(2) Lie algebra, this is a *faithful* representation of the quantum spin-1 operator. Then the model Hamiltonian can be expressed as:

$$H = \sum_{\mathbf{k},\sigma} \epsilon_{\mathbf{k}} C_{\mathbf{k},\sigma}^{\dagger} C_{\mathbf{k},\sigma} - \frac{J}{2}\left(\sqrt{2}d_1^{\dagger}C_{\uparrow} + d_0^{\dagger}C_{\downarrow}\right)\left(\sqrt{2}C_{\uparrow}^{\dagger}d_1 + C_{\downarrow}^{\dagger}d_0\right) - \frac{J}{2}\left(\sqrt{2}d_{-1}^{\dagger}C_{\downarrow} + d_0^{\dagger}C_{\uparrow}\right)\left(\sqrt{2}C_{\downarrow}^{\dagger}d_{-1} + C_{\uparrow}^{\dagger}d_0\right), \tag{4}$$

where an irrelevant potential term has been neglected. We emphasize that employing this pseudo-fermion representation for the spin-1 moment is *instrumental* to explicitly reveal the residual symmetry of the bound state formed in the strong coupling limit.

B. Effective resonant level model and impurity spectral function

In analogy with the functional integral approach for the spin-1/2 Kondo impurity model [10], a saddle point approximation can be adopted by defining an effective MF like variable:

$$\langle\sqrt{2}d_1^{\dagger}C_{\uparrow} + d_0^{\dagger}C_{\downarrow}\rangle = \langle\sqrt{2}d_{-1}^{\dagger}C_{\downarrow} + d_0^{\dagger}C_{\uparrow}\rangle \equiv -\sqrt{2}V, \tag{5}$$

where we assume the invariance of the low-energy excitations under the transformations $d_1 \Leftrightarrow d_{-1}$ and $C_{\uparrow} \Leftrightarrow C_{\downarrow}$. An effective resonant level model is then derived:

$$\begin{aligned} H_{eff} &= \sum_{\mathbf{k},\sigma} \epsilon_{\mathbf{k}} C_{\mathbf{k},\sigma}^{\dagger} C_{\mathbf{k},\sigma} + \frac{JV}{\sqrt{2N}} \sum_{\mathbf{k},\boldsymbol{\sigma}} \left(C_{\mathbf{k},\sigma}^{\dagger}d_0 + h.c.\right) \\ &+ \frac{JV}{\sqrt{N}} \sum_{\mathbf{k}} \left(C_{\mathbf{k},\uparrow}^{\dagger}d_1 + C_{\mathbf{k},\downarrow}^{\dagger}d_{-1} + h.c.\right) \\ &+ \lambda \sum_{\alpha} d_{\alpha}^{\dagger}d_{\alpha} + 2JV^2 - \lambda, \end{aligned} \tag{6}$$

where the constraint has been implemented by a Lagrange multiplier λ. In the effective resonant level model, $d_1^{\dagger}|0\rangle$ hybridizes with the spin-up electrons, $d_{-1}^{\dagger}|0\rangle$ with the spin-down electrons, while $d_0^{\dagger}|0\rangle$ hybridizes with both spin-up and -down electrons. Then the effective resonant level displays a Z_2 symmetry describing the invariance of the model under the transformations $d_1 \Leftrightarrow d_{-1}$ and $C_{\uparrow} \Leftrightarrow C_{\downarrow}$, i.e., an Ising symmetry. This property reflects the residual symmetry of the bound state in the strong coupling limit and the *quantum* nature of the partially screened moment.

Introducing a Nambu spinor to denote the impurity triplet state $\phi^{\dagger} = \left(d_1^{\dagger}, d_0^{\dagger}, d_{-1}^{\dagger}\right)$, we can derive the impurity retarded Green's function (GF) matrix as

$$\widehat{G}_d(\omega) = \begin{bmatrix} \omega-\lambda+i\Gamma & i\Gamma/\sqrt{2} & 0 \\ i\Gamma/\sqrt{2} & \omega-\lambda+i\Gamma & i\Gamma/\sqrt{2} \\ 0 & i\Gamma/\sqrt{2} & \omega-\lambda+i\Gamma \end{bmatrix}^{-1},$$

where $\Gamma = \pi\rho_f(JV)^2$ is a hybridization integral between the magnetic moment and the conduction electrons. The diagonal retarded GF is then derived,

$$\begin{aligned} G_1(\omega) &= \frac{(\omega-\lambda+i\Gamma)(\omega-\lambda+i\Gamma)+\Gamma/2}{(\omega-\lambda)(\omega-\lambda+i\Gamma)(\omega-\lambda+i2\Gamma)}, \\ G_0(\omega) &= \frac{(\omega-\lambda+i\Gamma)}{(\omega-\lambda)(\omega-\lambda+i2\Gamma)}, \\ G_{-1}(\omega) &= G_1(\omega), \end{aligned} \tag{7}$$

and non-zero off-diagonal retarded GFs are all equal to

$$G_{1,0}(\omega) = \frac{-i\Gamma/\sqrt{2}}{(\omega-\lambda)(\omega-\lambda+i2\Gamma)}. \tag{8}$$

By summing up the imaginary parts of the diagonal GFs, the impurity spectral function can thus be obtained

$$A_d(\omega) = \delta(\omega-\lambda) + \frac{1}{\pi}\left[\frac{\Gamma}{(\omega-\lambda)^2+\Gamma^2} + \frac{2\Gamma}{(\omega-\lambda)^2+4\Gamma^2}\right],$$

where an essential feature of the effective model has been displayed: two Lorentzian resonances are exhibited at $\omega = \lambda$ with half widths Γ and 2Γ, respectively; what is more, a sharp δ-resonance appears at $\omega = \lambda$. Unlike the two-channel spin-1/2 single Kondo impurity model, where partial impurity degrees of freedom decouple from

the conduction electrons leading to a zero fermionic mode [11], all three components of the moment here are coupled to the conduction electrons, and a sharp δ-resonance is induced by the remanent Z_2 Ising symmetry of the bound state. Using the spectral function, the impurity contribution to the free energy can be evaluated

$$\begin{aligned}\delta F &= -\frac{1}{\pi}\int_{-D}^{D} d\omega n_f(\omega)\left[\frac{\pi}{2}\mathrm{sgn}(\omega-\lambda)+\tan^{-1}\left(\frac{\Gamma}{\lambda-\omega}\right)\right.\\ &\left.+\tan^{-1}\left(\frac{2\Gamma}{\lambda-\omega}\right)\right]+2JV^2-\lambda, \end{aligned}\tag{9}$$

where $n_f(\omega) = (e^{\beta\omega}+1)^{-1}$ is the Fermi distribution function. At $T = 0$, the saddle point solution leads to $\lambda \approx 0$, indicating that the sharp δ- resonance and two Lorentzian resonances lie at the Fermi level with $\Gamma \approx D\exp\left(-\frac{2}{3\rho_f J}\right)$, where D is the half conduction electron bandwidth.

The contribution to the impurity entropy can be calculated using the relation $S = -(\partial F/\partial T)$. At $T = 0$, we find that $S_{\mathrm{imp}} = -k_B \ln 2$, implying that the magnetic moment has been partially screened by the conduction electrons. The total impurity entropy down to $T = 0$ will be $\Delta S_{\mathrm{imp}} = k_B \ln(3/2)$, being consistent with the exact result [12]. However, the impurity contribution to the specific heat is still linear in temperature, in spite of the δ-resonance appearing in the impurity spectral function at the Fermi level.

C. Dynamic spin susceptibilities and scattering T-matrices

To fully reveal the singularity in the effective resonant level model, we calculate the dynamic impurity spin correlation functions at finite temperatures. After some algebra, the leading order impurity spin dynamic spectral function is obtained

$$\begin{aligned}&\mathtt{Im}\chi_d^{zz}(\omega,T)\\ &= -\frac{\Gamma}{4}\left[\frac{1}{\omega^2+\Gamma^2}+\frac{1}{\omega^2+4\Gamma^2}\right]\tanh\left(\frac{\omega}{2k_BT}\right),\end{aligned}\tag{10}$$

and the corresponding real part is thus estimated as $\mathtt{Re}\chi_d^{zz}(\omega,T) \propto \ln(\max(\omega,T)/\Gamma)$. The transverse impurity spin dynamic susceptibility $\chi_d^{-+}(\omega,T)$ shows a similar behavior. Such a logarithmic divergence of the impurity spin susceptibility is reminiscent of the singularity in the overscreened two-channel single Kondo impurity model [11]. In some sense the two-channel overscreened and spin-1 underscreened cases are somehow "dual" to each other: in the former case the singularity is induced by the "extra" screening channel of conduction electrons, while in the latter case it is due to the "extra spin channel" of the impurity [6].

Now we derive the scattering T-matrix of the conduction electrons. By calculating $G_{\sigma,\sigma'}(\mathbf{k},\mathbf{k}',i\omega_n)$ through their equations of motion, the retarded T-matrices are derived as

$$\begin{aligned}T_{\sigma,\sigma}(\omega) &= V^2\left[G_1(\omega)+\sqrt{2}G_{1,0}(\omega)+\frac{1}{2}G_0(\omega)\right],\\ T_{\sigma,-\sigma}(\omega) &= V^2\left[\sqrt{2}G_{1,0}(\omega)+\frac{1}{2}G_0(\omega)\right],\end{aligned}\tag{11}$$

where the off-diagonal impurity GFs are involved. The scattering cross sections of the conduction electrons off the bound state are proportional to

$$\begin{aligned}\mathtt{Im}T_{\sigma,\sigma}(\omega) &= \frac{-1}{2\pi\rho_f}\left[\frac{\Gamma^2}{\omega^2+\Gamma^2}+\frac{4\Gamma^2}{\omega^2+4\Gamma^2}\right],\\ \mathtt{Im}T_{\sigma,-\sigma}(\omega) &= \frac{-1}{2\pi\rho_f}\left[-\frac{\Gamma}{2}\delta(\omega)+\frac{3\Gamma^2}{\omega^2+4\Gamma^2}\right].\end{aligned}\tag{12}$$

For the non-spin-flip scatterings, two Lorentzian resonances are obtained and the δ-resonance is exactly cancelled, while the δ-resonance appears in the spin-flip scattering processes where the residual magnetic moment of the bound state has to spin-flip as well. Thus, the remanent moment with Z_2 symmetry in the underscreened case gives rise to a singular behavior in both local impurity and conduction electrons properties.

Compared with the Bethe ansatz and NRG results [7], our resonant level model serves as an effective model at the singular Fermi liquid fixed point. Given the singular impurity spin dynamic spectral function, the retarded self-energy of conduction electrons due to exchange of impurity spin fluctuations will lead to

$$\Sigma_\sigma(\omega,T) \sim g^2\left(\omega\ln\frac{x}{D}-i\frac{\pi}{2}x\right),\tag{13}$$

where $x = \max(|\omega|,T)$ and g is a coupling constant. This is a kind of local marginal Fermi liquid behavior [13]. Furthermore, a logarithmic correction to the linear-in-temperature specific heat can also be obtained within the one-loop approximation.

D. Effects of the external magnetic field

In the presence of a magnetic field, an additional term $-hS^z$ lifts the Ising degeneracy so the singularity at the Fermi level is suppressed. The diagonal impurity retarded GFs are given by

$$\begin{aligned}G_1(\omega) &= \frac{(\omega-\lambda+i\Gamma)(\omega-\lambda-h+i\Gamma)+\Gamma^2/2}{(\omega-\lambda+i\Gamma)\left[(\omega-\lambda)^2+i2\Gamma(\omega-\lambda)-h^2\right]},\\ G_0(\omega) &= \frac{(\omega-\lambda+i\Gamma)^2-h^2}{(\omega-\lambda+i\Gamma)\left[(\omega-\lambda)^2+i2\Gamma(\omega-\lambda)-h^2\right]},\\ G_{-1}(\omega) &= \frac{(\omega-\lambda+i\Gamma)(\omega-\lambda+h+i\Gamma)+\Gamma^2/2}{(\omega-\lambda+i\Gamma)\left[(\omega-\lambda)^2+i2\Gamma(\omega-\lambda)-h^2\right]}.\end{aligned}$$

If the magnetic field is weak, i.e., $h \ll \Gamma$, the impurity spectral function exhibits three Lorentzian resonances at the same energy $\omega = \lambda$, with different half widths Γ, and $\left(\Gamma \pm \sqrt{\Gamma^2 - h^2}\right)$, while the δ-resonance disappears. At $T = 0$, $\lambda \approx 0$, and the impurity spin susceptibility is derived as

$$\chi_d \approx \frac{1}{\pi\Gamma}\left[\ln\left(\frac{2\Gamma}{h}\right) - 2\right], \tag{14}$$

which displays a logarithmic dependence on h, indicating a local quantum critical point at $T = 0$ and $h = 0$. When the magnetic field is strong enough, i.e., $h > \Gamma$, the impurity spectral function shows three separated Lorentzian resonances at $\omega = \lambda$ and $\omega = \lambda \pm \sqrt{h^2 - \Gamma^2}$, with the same half width Γ. For $h = \Gamma$, three Lorentzian resonances with a half width Γ reconcile again at $\omega = \lambda$.

III. EFFECTIVE MODEL FOR SPIN-1/2 TWO KONDO IMPURITY MODEL

The above described singular behavior in the underscreened spin-1 Kondo impurity model only arises when $S > 1/2$, while the real Kondo lattice systems usually involve spin-1/2 magnetic impurities. However, it is also possible for the underscreening to be an intrinsic feature around the quantum critical point [3]. The simplest model for such a study is a spin-1/2 two magnetic Kondo impurity model [14, 15],

$$H = \sum_{\mathbf{k},\sigma} \epsilon_{\mathbf{k}} C^\dagger_{\mathbf{k},\sigma} C_{\mathbf{k},\sigma} + J\left[\mathbf{S}_1 \cdot \mathbf{s}(\mathbf{r}_1) + \mathbf{S}_2 \cdot \mathbf{s}(\mathbf{r}_2)\right] + I\mathbf{S}_1 \cdot \mathbf{S}_2, \tag{15}$$

where $\mathbf{S}_1$ and $\mathbf{S}_2$ are localized spin-1/2 moments set at $\mathbf{r}_1 = \mathbf{R}/2$ and $\mathbf{r}_2 = -\mathbf{R}/2$, respectively, the Kondo coupling is antiferromagnetic $J > 0$, and a direct inter-impurity interaction I is included. When the inter-impurity antiferromagnetic coupling I/T_k is very large (T_k is the single impurity Kondo temperature), two spin-1/2 impurities lock into a singlet state, and there is no Kondo effect and the conduction electrons are completely unaffected by the impurities. Conversely, for a large and ferromagnetic coupling I/T_k, the two impurities become an effective $S = 1$ magnetic impurity, and a fully screened Kondo behavior occurs at low temperatures due to the presence of the two conduction electron channels. However, the most intriguing behavior, as shown by the numerical RG studies,[14] appears in-between these two stable limiting phases, at a plausible quantum critical point. Namely, the impurity singlet and triplet states become *degenerate* at a critical value of the inter-impurity coupling $I_c \sim 2.2T_K$, displaying a local quantum critical behavior with partially screened moment.

A. Coupled representation for the spin-1/2 impurities

Using the SU(2) pseudo-fermion representation for the spin-1/2 impurities, the Kondo spin exchange interactions are written in the Coqblin-Schrieffer form,

$$\begin{aligned} H &= \sum_{\mathbf{k},\sigma} \epsilon_{\mathbf{k}} C^\dagger_{\mathbf{k},\sigma} C_{\mathbf{k},\sigma} + \frac{I}{2}\sum_{\sigma,\sigma'} d^\dagger_{1,\sigma} d_{1,\sigma'} d^\dagger_{2,\sigma'} d_{2,\sigma} \\ &\quad - \frac{J}{2}\sum_{\sigma,\sigma'}\left(d^\dagger_{1,\sigma} d_{1,\sigma'} C_{\mathbf{r}_1,\sigma} C^\dagger_{\mathbf{r}_1,\sigma'} + d^\dagger_{2,\sigma} d_{2,\sigma'} C_{\mathbf{r}_2,\sigma} C^\dagger_{\mathbf{r}_2,\sigma'}\right), \end{aligned}$$

where the potential scattering terms have been neglected. Moreover, two constraints $\sum_\sigma d^\dagger_{1,\sigma} d_{1,\sigma} = 1$ and $\sum_\sigma d^\dagger_{2,\sigma} d_{2,\sigma} = 1$ have to be imposed. In general, the two spin-1/2 operators can also be represented by four coupled states

$$\begin{aligned} |\uparrow;\uparrow\rangle &= f^\dagger_1|0\rangle, |\uparrow;\downarrow\rangle = f^\dagger_2|0\rangle, \\ |\downarrow;\uparrow\rangle &= f^\dagger_3|0\rangle, |\downarrow;\downarrow\rangle = f^\dagger_4|0\rangle, \end{aligned}$$

which can be described by a local four-component fermion and the constraints are replaced by $\sum_\alpha f^\dagger_\alpha f_\alpha = 1$. Using the projection procedure, the two impurity Kondo model can be expressed as

$$\begin{aligned} H &= \sum_{\mathbf{k},\sigma} \epsilon_{\mathbf{k}} C^\dagger_{\mathbf{k},\sigma} C_{\mathbf{k},\sigma} - \frac{J}{2}\Big[\left(f^\dagger_1 C_{\mathbf{r}_1,\uparrow} + f^\dagger_3 C_{\mathbf{r}_1,\downarrow}\right)\left(C^\dagger_{\mathbf{r}_1,\uparrow} f_1 + C^\dagger_{\mathbf{r}_1,\downarrow} f_3\right) + \left(f^\dagger_2 C_{\mathbf{r}_1,\uparrow} + f^\dagger_4 C_{\mathbf{r}_1,\downarrow}\right)\left(C^\dagger_{\mathbf{r}_1,\uparrow} f_2 + C^\dagger_{\mathbf{r}_1,\downarrow} f_4\right) \\ &\quad + \left(f^\dagger_1 C_{\mathbf{r}_2,\uparrow} + f^\dagger_2 C_{\mathbf{r}_2,\downarrow}\right)\left(C^\dagger_{\mathbf{r}_2,\uparrow} f_1 + C^\dagger_{\mathbf{r}_2,\downarrow} f_2\right) + \left(f^\dagger_3 C_{\mathbf{r}_2,\uparrow} + f^\dagger_4 C_{\mathbf{r}_2,\downarrow}\right)\left(C^\dagger_{\mathbf{r}_2,\uparrow} f_3 + C^\dagger_{\mathbf{r}_2,\downarrow} f_4\right)\Big] \\ &\quad + \frac{I}{2}\left(f^\dagger_1 f_1 + f^\dagger_4 f_4 + f^\dagger_2 f_3 + f^\dagger_3 f_2\right), \end{aligned} \tag{16}$$

where the direct inter-impurity coupling has been transformed into a quadratic form, and can be considered exactly.

B. Effective resonant level model

In order to derive an effective model to describe the local quantum critical point, we employ a similar method as in the functional integral approach for the spin-1/2 Kondo impurity model [10], and a saddle point solution can be

deduced by introducing an effective hybridization amplitude:

$$\langle f_1^\dagger C_{\mathbf{r}_1,\uparrow} + f_3^\dagger C_{\mathbf{r}_1,\downarrow}\rangle = \langle f_2^\dagger C_{\mathbf{r}_1,\uparrow} + f_4^\dagger C_{\mathbf{r}_1,\downarrow}\rangle = \langle f_1^\dagger C_{\mathbf{r}_2,\uparrow} + f_2^\dagger C_{\mathbf{r}_2,\downarrow}\rangle = \langle f_3^\dagger C_{\mathbf{r}_2,\uparrow} + f_4^\dagger C_{\mathbf{r}_2,\downarrow}\rangle = -V,$$

where the spin rotational symmetry and parity symmetry between the magnetic impurities ($\mathbf{S}_1 \Leftrightarrow \mathbf{S}_2$) have been assumed. Using linear combinations of the impurity spin anti-parallel states, $\widetilde{f}_2 = (f_2+f_3)/\sqrt{2}$ and $\widetilde{f}_3 = (f_2-f_3)/\sqrt{2}$, an effective resonant level model can be derived:

$$\begin{aligned} H_{eff} = &\sum_{\mathbf{k},\sigma} \epsilon_{\mathbf{k}} C_{\mathbf{k},\sigma}^\dagger C_{\mathbf{k},\sigma} + \frac{JV}{\sqrt{2N}} \sum_{\mathbf{k},\boldsymbol{\sigma}} \left(C_{\mathbf{k},\sigma}^\dagger \widetilde{f}_2 \cos\frac{\mathbf{k}\cdot\mathbf{R}}{2} + h.c.\right) + \frac{JV}{\sqrt{N}} \sum_{\mathbf{k}} \left[\left(C_{\mathbf{k},\uparrow}^\dagger f_1 + C_{\mathbf{k},\downarrow}^\dagger f_4 \right) \cos\frac{\mathbf{k}\cdot\mathbf{R}}{2} + h.c.\right] \\ &- \frac{JV}{\sqrt{2N}} \sum_{\mathbf{k},\boldsymbol{\sigma}} \left(i\sigma C_{\mathbf{k},\sigma}^\dagger \widetilde{f}_3 \sin\frac{\mathbf{k}\cdot\mathbf{R}}{2} + h.c.\right) + (\lambda - I/2)\, \widetilde{f}_3^\dagger \widetilde{f}_3 + (\lambda + I/2) \left(f_1^\dagger f_1 + f_4^\dagger f_4 + \widetilde{f}_2^\dagger \widetilde{f}_2 \right) + (2JV^2 - \lambda), \end{aligned} \tag{17}$$

where the local constraint has been implemented by a Lagrange multiplier λ. Then the conduction electrons in three spatial dimension can be reduced and divided into symmetric and antisymmetric channels, defined by

$$C_{k,+,\sigma} = \frac{1}{\sqrt{N_+(k)}} \int \frac{d\Omega_{\mathbf{k}}}{4\pi} C_{\mathbf{k},\sigma} \cos\frac{\mathbf{k}\cdot\mathbf{R}}{2}, \quad C_{k,-,\sigma} = \frac{i}{\sqrt{N_-(k)}} \int \frac{d\Omega_{\mathbf{k}}}{4\pi} C_{\mathbf{k},\sigma} \sin\frac{\mathbf{k}\cdot\mathbf{R}}{2}, \tag{18}$$

where $N_\pm(k) = \frac{1}{2}\left(1 \pm \sin kR/(kR)\right)$ and the effective resonant level model becomes a one-dimensional system with two separated conduction electron channels interacting with two magnetic impurities $H_{eff} = H_+ + H_- + (2JV^2 - \lambda)$, where

$$\begin{aligned} H_+ &= \sum_k \epsilon_k C_{k,+,\sigma}^\dagger C_{k,+,\sigma} + \frac{JV}{\sqrt{N}} \sum_k \sqrt{N_+(k)} \left[\left(C_{k,+,\uparrow}^\dagger f_1 + C_{k,+,\downarrow}^\dagger f_4 \right) + h.c.\right] \\ &\quad + \frac{JV}{\sqrt{2N}} \sum_{k,\boldsymbol{\sigma}} \sqrt{N_+(k)} \left(C_{k,+,\sigma}^\dagger \widetilde{f}_2 + h.c.\right) + (\lambda + I/2) \left(f_1^\dagger f_1 + f_4^\dagger f_4 + \widetilde{f}_2^\dagger \widetilde{f}_2 \right), \\ H_- &= \sum_k \epsilon_k C_{k,-,\sigma}^\dagger C_{k,-,\sigma} - \frac{JV}{\sqrt{2N}} \sum_{k,\boldsymbol{\sigma}} \sqrt{N_-(k)} \left(\sigma C_{k,-,\sigma}^\dagger \widetilde{f}_3 + h.c.\right) + (\lambda - I/2)\, \widetilde{f}_3^\dagger \widetilde{f}_3. \end{aligned} \tag{19}$$

It is clearly seen that $\widetilde{f}_3^\dagger|0\rangle$ describes the impurity singlet state with energy $(\lambda - I/2)$, and hybridizes with the *antisymmetric* channel of the conduction electrons, while $f_1^\dagger|0>$, $f_4^\dagger|0>$, and $\widetilde{f}_2^\dagger|0>$ describe the impurity triplet states with energy $(\lambda + I/2) = \epsilon_f$ and couple to the *symmetric* channel of the conduction electrons. The effective resonant level model in the symmetric channel shares a *similar* form of the effective model as for the isotropic underscreened spin-1 Kondo impurity model, except for the momentum dependence of the hybridization integrals.

C. Impurity spectral function

Now the effective Hamiltonian can be diagonalized as before, and the retarded impurity quasiparticle GFs are obtained:

$$\begin{aligned} G_1(\omega) &= G_4(\omega) = \frac{1/4}{\omega - \epsilon_f} + \frac{1/4}{\omega - \epsilon_f - 2\Delta_+ + 2i\Gamma_+} \\ &\quad + \frac{1/2}{\omega - \epsilon_f - \Delta_+ + i\Gamma_+}, \\ G_2(\omega) &= \frac{1/2}{\omega - \epsilon_f} + \frac{1/2}{\omega - \epsilon_f - 2\Delta_+ + 2i\Gamma_+}, \\ G_3(\omega) &= \frac{1}{\omega - \epsilon_f + I - \Delta_- + i\Gamma_-}, \end{aligned} \tag{20}$$

where the self-energy corrections are involved

$$\begin{aligned} \Delta_\pm(\omega) &= \frac{(JV)^2}{N} \sum_k \frac{N_\pm(k)}{\omega - \epsilon_k}, \\ \Gamma_\pm &= \pi\rho(k_f) N_\pm(k_f)(JV)^2. \end{aligned} \tag{21}$$

Thus, the impurity quasiparticle spectral function is given by the imaginary parts of the retarded GFs, i.e.

$$A_{\mathrm{imp}}(\omega) = \delta(\omega - \epsilon_f) + \frac{\Gamma_+/\pi}{(\omega - \epsilon_f - \Delta_+)^2 + \Gamma_+^2} + \frac{2\Gamma_+/\pi}{(\omega - \epsilon_f - 2\Delta_+)^2 + 4\Gamma_+^2} + \frac{\Gamma_-/\pi}{(\omega - \epsilon_f + I - \Delta_-)^2 + \Gamma_-^2}, \tag{22}$$

where four resonances appear in the impurity spectral function, and the δ-resonance persists at the impurity energy level $\omega = \epsilon_f$, leading to a singular behavior for the low energy quasiparticles.

When the inter-impurity coupling is antiferromagnetic $I > 0$, the impurity singlet state is the lowest energy state, while for the ferromagnetic inter-impurity interaction $I < 0$, the impurity triplet state has the lowest energy. In general, the energy levels of both the impurity singlet and triplet states should be *strongly* renormalized by both the inter-impurity interaction and the couplings with the conduction electrons. Such a renormalization effects on the impurity energy levels are not fully considered in the present treatments. However, in the symmetric channel of the effective model, we have found a δ-resonance singularity corresponding to the partially screened impurity triplet state, which is similar to what we find in the underscreened spin-1 Kondo impurity model. Therefore, we believe that the singular behavior of the spin-1/2 two Kondo impurity model around the nontrivial quantum critical point is closely related to the low-energy physics of the spin-1 underscreened Kondo model. This indicates that the peculiar behavior observed in a large class of heavy fermion metals[2, 3] might be related to the physics of underscreened Kondo model.

IV. QUANTUM DOTS WITH EVEN NUMBER OF ELECTRONS

To experimentally observe the singular behavior inherent to the underscreened spin-1 Kondo impurity model, the mesoscopic quantum dot systems with even number of electrons are among the promising candidates [16, 17]. In the presence of a large Hund's rule coupling between two topmost dot electrons, an effective two coupled spin-1/2 Kondo impurity model has been derived by Kikoin and Avishai [18].

$$H = \sum_{\mathbf{k},\sigma} \epsilon_{\mathbf{k}} C^\dagger_{\mathbf{k},\sigma} C_{\mathbf{k},\sigma} + (J_1 \mathbf{S}_1 + J_2 \mathbf{S}_2) \cdot \mathbf{s}(\mathbf{0}) - I \mathbf{S}_1 \cdot \mathbf{S}_2, \tag{23}$$

where J_1 and J_2 are two positive antiferromagnetic Kondo couplings, the Hund's coupling I is ferromagnetic, and the two magnetic moments are sitting on the same site. Using the SU(2) pseudo-fermion representation for the spin-1/2 operators, the Kondo spin exchanges are written in the Coqblin-Schrieffer form,

$$\begin{aligned} H &= \sum_{\mathbf{k},\sigma} \epsilon_{\mathbf{k}} C^\dagger_{\mathbf{k},\sigma} C_{\mathbf{k},\sigma} - \frac{I}{2} \sum_{\sigma,\sigma'} d^\dagger_{1,\sigma} d_{1,\sigma'} d^\dagger_{2,\sigma'} d_{2,\sigma} \\ &\quad - \frac{1}{2} \sum_{\sigma,\sigma'} \left(J_1 d^\dagger_{1,\sigma} d_{1,\sigma'} + J_2 d^\dagger_{2,\sigma} d_{2,\sigma'} \right) C_\sigma C^\dagger_{\sigma'} \end{aligned} \tag{24}$$

where the potential scattering terms have been neglected. Two single occupied constraints $\sum_\sigma d^\dagger_{1,\sigma} d_{1,\sigma} = 1$ and $\sum_\sigma d^\dagger_{2,\sigma} d_{2,\sigma} = 1$ are imposed. The two spin-1/2 operators can also be represented by four states $|\uparrow;\uparrow\rangle = f^\dagger_1 |0\rangle$, $|\uparrow;\downarrow\rangle = f^\dagger_2 |0\rangle$, $|\downarrow;\uparrow\rangle = f^\dagger_3 |0\rangle$, $|\downarrow;\downarrow\rangle = f^\dagger_4 |0\rangle$ and the constraints are replaced by $\sum_\alpha f^\dagger_\alpha f_\alpha = 1$. Then the model can be expressed as

$$\begin{aligned} H &= \sum_{\mathbf{k},\sigma} \epsilon_{\mathbf{k}} C^\dagger_{\mathbf{k},\sigma} C_{\mathbf{k},\sigma} - \frac{J_1}{2} \left[\left(f^\dagger_1 C_\uparrow + f^\dagger_3 C_\downarrow \right) \left(C^\dagger_\uparrow f_1 + C^\dagger_\downarrow f_3 \right) + \left(f^\dagger_2 C_\uparrow + f^\dagger_4 C_\downarrow \right) \left(C^\dagger_\uparrow f_2 + C^\dagger_\downarrow f_4 \right) \right] \\ &\quad - \frac{J_2}{2} \left[\left(f^\dagger_1 C_\uparrow + f^\dagger_2 C_\downarrow \right) \left(C^\dagger_\uparrow f_1 + C^\dagger_\downarrow f_2 \right) + \left(f^\dagger_3 C_\uparrow + f^\dagger_4 C_\downarrow \right) \left(C^\dagger_\uparrow f_3 + C^\dagger_\downarrow f_4 \right) \right] - \frac{I}{2} \left(f^\dagger_1 f_1 + f^\dagger_4 f_4 + f^\dagger_2 f_3 + f^\dagger_3 f_2 \right), \end{aligned} \tag{25}$$

Actually, using an SU(4) pseudo-fermion representation, both spin-1/2 operators $\mathbf{S}_1$ and $\mathbf{S}_2$ are expressed jointly [19], and the same form of the model Hamiltonian can be obtained.

A. Effective model Hamiltonian

Implementing the constraint by a Lagrangian multiplier λ and introducing two effective hybridization variables: $\langle f^\dagger_1 C_\uparrow + f^\dagger_3 C_\downarrow \rangle = \langle f^\dagger_2 C_\uparrow + f^\dagger_4 C_\downarrow \rangle = -v_1$ and $\langle f^\dagger_1 C_\uparrow + f^\dagger_2 C_\downarrow \rangle = \langle f^\dagger_3 C_\uparrow + f^\dagger_4 C_\downarrow \rangle = -v_2$, the strong coupling MF approximation can be carried out as before. With linear combinations of the impurity spin antiparallel states, $\widetilde{f}_2 = (f_2 + f_3)/\sqrt{2}$ and $\widetilde{f}_3 = (f_2 - f_3)/\sqrt{2}$, a modified effective resonant level model can be derived:

$$H_{eff} = \sum_{\mathbf{k},\sigma} \epsilon_{\mathbf{k}} C^{\dagger}_{\mathbf{k},\sigma} C_{\mathbf{k},\sigma} + \frac{V}{\sqrt{2N}} \sum_{\mathbf{k},\boldsymbol{\sigma}} \left(C^{\dagger}_{\mathbf{k},\sigma} \widetilde{f}_2 + h.c. \right) + \frac{V}{\sqrt{N}} \sum_{\mathbf{k}} \left(C^{\dagger}_{\mathbf{k},\uparrow} f_1 + C^{\dagger}_{\mathbf{k},\downarrow} f_4 + h.c. \right)$$
$$+ \frac{Vr}{\sqrt{2N}} \sum_{\mathbf{k},\boldsymbol{\sigma}} \left(\sigma C^{\dagger}_{\mathbf{k},\sigma} \widetilde{f}_3 + h.c. \right) + (\epsilon_f + I)\, \widetilde{f}^{\dagger}_3 \widetilde{f}_3 + \epsilon_f \left(f^{\dagger}_1 f_1 + f^{\dagger}_4 f_4 + \widetilde{f}^{\dagger}_2 \widetilde{f}_2 \right) + (J_1 v_1^2 + J_2 v_2^2 - \lambda), \quad (26)$$

where $V = (J_1 v_1 + J_2 v_2)/2$, $r = (J_1 v_1 - J_2 v_2)/(J_1 v_1 + J_2 v_2)$, $\epsilon_f = \lambda - I/2$, and only one conduction electron channel effectively couples to the dot electrons. It is clearly seen that $\widetilde{f}^{\dagger}_3 |0\rangle$ describes the impurity singlet state with energy $(\epsilon_f + I)$, and hybridizes with the spin-up and -down conduction electrons, while the impurity triplet state with energy ϵ_f couples to the conduction electrons as discussed above. Since the inter-impurity ferromagnetic coupling I is large enough, the impurity singlet energy level lies far above ϵ_f while the triplet state lies at ϵ_f. The effective resonant level model in the limit of $J_1 = J_2$ reduces to the effective model for the isotropic underscreened spin-1 Kondo impurity model in the strong coupling limit, where the impurity singlet state completely decouples from the conduction electrons.

B. Dot electron spectral function and spin susceptibilities

Now the effective Hamiltonian is diagonalized, and the dot electron spectral function is thus given by

$$A_{\rm dot}(\omega) = \delta\left(\omega - \epsilon_f\right) + \frac{1}{\pi} \frac{2\Gamma}{\left(\omega - \epsilon_f\right)^2 + 4\Gamma^2} + \frac{1}{\pi} \frac{\Gamma \left[(1 + r^2) \left(\omega - \epsilon_f\right)^2 - 2I \left(\omega - \epsilon_f\right) + I^2 \right]}{\left(\omega - \epsilon_f\right)^2 \left(\omega - \epsilon_f - I\right)^2 + \Gamma^2 \left[(1 + r^2) \left(\omega - \epsilon_f\right) - I \right]^2}, \quad (27)$$

where four resonances appear in the dot spectral function, and the δ-resonance persists at $\omega = \epsilon_f$, leading to a singular behavior for the dot electrons the same way as in the underscreened spin-1 Kondo impurity model. Since the uniform spin and staggered spin density operators are expressed as

$$\begin{aligned} (S^z_1 + S^z_2) &= f^{\dagger}_1 f_1 - f^{\dagger}_4 f_4, \\ (S^z_1 - S^z_2) &= \widetilde{f}^{\dagger}_2 \widetilde{f}_3 + \widetilde{f}^{\dagger}_3 \widetilde{f}_2, \end{aligned} \quad (28)$$

the corresponding spin susceptibilities can be evaluated and found: $\mathtt{Im}\chi^u_{\rm imp}(\omega, T)$, $\mathtt{Im}\chi^s_{\rm imp}(\omega, T) \propto \tanh\left(\omega/(2k_B T)\right)$, from which the corresponding real part dynamic susceptibilities display a logarithmic dependence on $\max(\omega, T)$ as for the spin-1 underscreened Kondo impurity model. We can also show that the singularity of the δ-resonance is only associated with the triplet state. Thus, we can interpret the large zero-bias anomalies of the differential conductance experimentally observed on the quantum dot with even occupied electrons without a magnetic field [20] as a manifestation of the residual Z_2 Ising degeneracy of the bound state composed of the triplet dot electron state with the conduction electrons in the leads.

V. CONCLUSION

To conclude, by proposing an effective resonant level model in the strong coupling limit for the spin-1 underscreened Kondo impurity model, we have shown that a local quantum critical behavior (logarithmic divergence of the local dynamic spin susceptibility) is induced by the formation of a bound state with a partially screened magnetic moment. We believe this is a *generic* feature of all underscreened Kondo models. The *quantum* nature of the remanent magnetic moment is explicitly exhibited through the symmetry determined degeneracy. A direct experimental observation of this quantum critical behavior might be possible in the quantum dot systems with even occupied electrons, and its implications related to some peculiar properties of f-electron heavy fermion systems are also indicated through the exploration of the spin-1/2 two Kondo impurity model.

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